studied from X-ray powder photograph. It is found that the dehydrated product consists of the double salt $Cu[(NH_4)SO_4]_2$, 2_2H_2O. Application of Lipson's method (Lipson, 1949) shows that it has an orthorhombic unit cell having dimensions: $a = 14.84$Å, $b = 12.52$Å, $c = 10.69$Å containing 8 molecules per cell. Conditions of reflection suggest the possibility of assigning to the dihydrate either of the space-group $P_{mn}\,2_1$ or P_{mnm}.

Since direct X-ray data on $Cu[(NH_4)SO_4]_2 6H_2O$ single crystal is lacking, we also undertook to study it and find that the hexahydrate which belongs to the space-group $P2_1/a$ and contains 2 molecules in the unit cell (Hofmann, 1931), has the following cell dimensions . $a = 9.27$ Å, $b = 12.50$Å, $c = 6.33$ Å, $\beta = 106.5'$.

It is interesting to note that the b axis in both the hexa- and dihydrate has the same length. It is, therefore, probable that the transition from the monoclinic to the orthorhombic system has taken place after merely a loss of 4 water molecules and a rearrangement of the molecules with reference to two vertical planes i.e., the transition is "topotactic" in nature.

Phase transition study for further dehydration and a more detailed study of structural changes by growing single crystals at high temperatures are under progress.

The author expresses her sincere thanks to Prof. A. Bose, D.Sc., F.N.I., for his kind interest and constant guidance and to Mr. S Ray, M.Sc., for many helpful discussions during the progress of the work.

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F-G MATRIX ELEMENTS FOR PYRAMIDAL XY_2Z MOLECULES

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(*Received July* 7, 1960)

Using Wilson's F-G matrix methods (1939, 1941), Pistorius (1959) obtained the elements for the planar XY_2Z type molecules employing the most general harmonic force field. These were recalculated by the authors (1960) and utilised to calculate the potential constants for certain specific cases. Venkateswarlu and Sundaram (1957) carried out a normal coordinate treatment for the pyramidal

XY_2Z type molecules neglecting a number of force constants. As a large number of these molecules are known and as their structural constants are being found by microwave techniques, it is felt desirable to carry out a similar calculation for this type of molecules employing the most general harmonic force field.

The following symmetry coordinates are set up which transform according to the characters of the corresponding vibration types.

$$A' \quad : \quad R_1 = \frac{1}{\sqrt{3}}(\Delta D+\Delta d_1+\Delta d_2)$$

$$R_2 = \frac{1}{\sqrt{6}}(2\Delta D-\Delta d_1-\Delta d_2)$$

$$R_3 = \frac{d}{\sqrt{3}}(\Delta\alpha_1+\Delta\alpha_2+\Delta\beta)$$

$$R_4 = \frac{d}{\sqrt{6}}(2\Delta\beta-\Delta\alpha_1-\Delta\alpha_2)$$

$$A'' \quad : \quad R_5 = \frac{1}{\sqrt{2}}(\Delta d_1-\Delta d_2)$$

$$R_6 = \frac{d}{\sqrt{2}}(\Delta\alpha_1-\Delta\alpha_2)$$

Here ΔD and Δd represent the $X-Z$ and $X-Y$ stretchings, $\Delta\alpha$ and $\Delta\beta$ the valence angle bendings of $Y-X-Z$ and $Y-X-Y$ respectively

The potential energy V is given by

$$\begin{aligned}2V &= f_D\,.\,\Delta D^2+f_d\sum_i\Delta d^2_i+2f_{Dd}\,.\,\Delta D\sum_i\Delta d_i\\ &+2f'_{dd}\Delta d_1\Delta d_2+2f_{D\alpha}\Delta D\;d\sum_i\Delta\alpha_i+2f_{d\alpha}\,.\,d\,.\sum_i\Delta d_i\Delta\alpha_i\\ &+2f'_{\alpha\alpha}\,.\,d\sum_{i\neq j}\Delta d_i\Delta\alpha_j+2f_{d\beta}d\Delta\beta\sum_i\Delta d_i\\ &+2f_{D\beta}\Delta D\,.\,d\Delta\beta+f_\alpha d^2\sum_i\Delta\alpha^2_i+2f_{\alpha\alpha}d^2\Delta\alpha_1\Delta\alpha_2\\ &+2f_{\alpha\beta}d^2\Delta\beta\sum_i\Delta\alpha_i+f_\beta d^2\Delta\beta^2\end{aligned}$$

The following F matrix elements are obtained :

$$A' \quad : \quad F_{11} = \frac{1}{3}(f_D+4f_{Dd}+2f_1)$$

$$F_{12} = \frac{1}{3\sqrt{2}}(2f_D+2f_{Dd}-2f_1)$$

$$F_{13} = \frac{1}{3}\ (2f_{D\alpha}+f_{D\beta}+2f_2+2f_{d\beta})$$

$$F_{14} = \frac{1}{3\sqrt{2}}(2f_{D\beta}+4f_{d\beta}-2f_{D\alpha}-2f_2)$$

$$F_{22} = \frac{1}{6}\ (4f_D-8f_{Dd}+2f_1)$$

$$\frac{1}{3\sqrt{2}}$$

$$F_{24} = \frac{1}{6}\ (4f_{D\beta}-4f_{D\alpha}+2f_2-4f_{d\beta})$$

$$F_{33} = \frac{1}{3}\ (2f_3+4f_{\alpha\beta}+f_\beta)$$

$$F_{34} = \frac{1}{3\sqrt{2}}\ (2f_{\alpha\beta}+2f_\beta-2f_3)$$

$$F_{44} = \frac{1}{6}\ (4f_\beta+2f_3-8f_{\alpha\beta})$$

Where f_1, f_2 and f_3 stand for

(f_d+f_{dd}), $(f_{d\alpha}+f'_{d\alpha})$ and $(f_\alpha+f_{\alpha\alpha})$ respectively.

A'' :

$$F_{55} = f_d-f_{dd}$$
$$F_{56} = f_{d\alpha}-f'_{d\alpha}$$
$$F_{66} = f_\alpha-f_{\alpha\alpha}$$

The elements of the inverse kinetic energy (G) matrix are given below using the following abbreviations :

$d/D-\cos\alpha = K$	$1+\cos\alpha+\cos\beta = Q$
$1-d/D\cos\alpha = L$	$1+\cos\beta-2\cos\alpha = T$
$1-\cos\alpha = M_\alpha$	$1+\cos\beta-2\cos^2\alpha = V$
$1-\cos\beta = M_\beta$	$\cos\alpha = c_\alpha$, $\sin\alpha = S_\alpha$
$1+\cos\beta = N$	
$1+2\cos\alpha = P$	$\cos\beta = C_\beta$, $\sin\beta = S_\beta$

μ_i = Reciprocal mass of the atom i

A' :

$$G_{11} = \frac{1}{3}\left[\mu_x\{2(N+P)-1\}+2\mu_y+\mu_z\right]$$

$$G_{12} = \frac{\sqrt{2}}{3}\left[\mu_x(P-Q)-\mu_y+\mu_z\right]$$

$$G_{13} = -\frac{2}{3}\,\mu_x \left[\frac{KQ+LP}{S_\alpha} + \frac{2M_\beta Q}{S_\beta}\right]$$

$$G_{14} = -\frac{\sqrt{2}}{3}\,\mu_x \left[\frac{KQ+LP}{S_\alpha} + 2\,\frac{S_\beta{}^2 + C_\alpha M_\beta}{S_\beta}\right]$$

$$G_{22} = \frac{1}{3}\,[\,\mu_x(2T+M_\beta) + \mu_y + 2\mu_z]$$

$$G_{23} = \frac{\sqrt{2}}{3}\,\mu_x \left[\frac{KT-2LM_\alpha}{S_\alpha} + \frac{M_\beta T}{S_\beta}\right]$$

$$G_{24} = \frac{1}{3}\,\mu_x \left[\frac{KT-2LM_\alpha}{S_\alpha} + \frac{2M_\beta T}{S_\beta}\right]$$

$$G_{33} = \frac{2}{3}\left[\mu_x \left\{\frac{K^2N+2L^2+4C_\alpha KL}{S_\alpha{}^2} + M_\beta + \frac{2M_\beta NK + 8C_\alpha M_\beta L}{S_\alpha S_\beta}\right\} + 2\mu_y\left(1+\frac{C_\alpha M_\beta}{S_\alpha S_\beta}\right) + \mu_z \frac{d^2}{D^2}\frac{V}{S_\alpha{}^2}\right]$$

$$G_{34} = \frac{\sqrt{2}}{3}\left[\mu_x \left\{2M_\beta + \frac{S_\beta{}^2K+2C_\alpha ML}{S_\alpha S_\beta} - \frac{NL^2+2L^2+4C_\alpha KL}{S_\alpha{}^2}\right\} + \mu_y - \mu_z \frac{d^2}{D^2} V\right]$$

$$G_{44} = \frac{1}{3}\left[\mu_x \left\{4M_\beta + \frac{M_\beta K^2+2L^2+4C_\alpha KL}{S_\alpha{}^2} - 4\,\frac{S_\beta{}^2K+2C_\alpha ML}{S_\alpha S_\beta}\right\} + \mu_y\left(5-\frac{4C_\alpha M_\beta}{S_\alpha S_\beta}\right) + \mu_z \frac{d^2}{D^2}\frac{V}{S_\alpha{}^2}\right]$$

$$G_{55} = \mu_x M_\beta + \mu_y$$

$$G_{56} = -\mu_x \frac{M_\beta K}{S_\alpha}$$

$$G_{66} = \mu_x \frac{M_\beta K}{S_\alpha{}^2} + \mu_y + \mu_z \frac{d^2}{D^2}\frac{M_\beta}{S_\alpha{}^2}$$

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